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09/502,133	02/11/2000	Harold E. Helson	103544.131US2	4787

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WILMERHALE/BOSTON
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EXAMINER	
JONES, HUGH M	

ART UNIT	PAPER NUMBER
2128	

NOTIFICATION DATE	DELIVERY MODE
05/25/2010	ELECTRONIC

Please find below and/or attached an Office communication concerning this application or proceeding.

The time period for reply, if any, is set in the attached communication.

Notice of the Office communication was sent electronically on above-indicated "Notification Date" to the following e-mail address(es):

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Office Action Summary	Application No.	Applicant(s)	
	09/502,133	HELSON, HAROLD E.	
	Examiner	Art Unit	
	Hugh Jones	2128	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE *3* MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

1)☒ Responsive to communication(s) filed on *3/2/2010*.

2a)☐ This action is **FINAL**. 2b)☒ This action is non-final.

3)☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

4)☒ Claim(s) *1,9 and 13-35* is/are pending in the application.

4a) Of the above claim(s) _____ is/are withdrawn from consideration.

5)☐ Claim(s) _____ is/are allowed.

6)☒ Claim(s) *1, 9, 13-35* is/are rejected.

7)☐ Claim(s) _____ is/are objected to.

8)☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

9)☐ The specification is objected to by the Examiner.

10)☒ The drawing(s) filed on *11 February 2000* is/are: a)☒ accepted or b)☐ objected to by the Examiner.

Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).

Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).

11)☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

12)☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).

a)☐ All b)☐ Some * c)☐ None of:

1.☐ Certified copies of the priority documents have been received.

2.☐ Certified copies of the priority documents have been received in Application No. _____.

3.☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

* See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

1) ☐ Notice of References Cited (PTO-892)
2) ☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)
3) ☐ Information Disclosure Statement(s) (PTO/SB/08) Paper No(s)/Mail Date _____.
4) ☐ Interview Summary (PTO-413) Paper No(s)/Mail Date. _____ .
5) ☐ Notice of Informal Patent Application
6) ☐ Other: _____.

DETAILED ACTION

1. Claims 1, 9, 13-35 of U. S. Patent 09/502,133 are in front of the office for consideration and remain pending. Claims 2-8, 10-12 are canceled.

2. Novel material is identified.

Claim Interpretation

3. Claim 1, for example, only requires:

> 1. (currently amended) A computer-implemented method for use in deriving a chemical structure diagram, comprising:
>
> identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;
>
> wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;
>
> laying out symmetrically equivalent atoms and bonds in the chemical structure diagram to visually express the identified symmetry in a stylized two-dimensional pictorial representation of the chemical structure; and
>
> outputting [[a]]the pictorial representation of the chemical structure.

The claim does not specify any special meaning to 'stylized'. The claim does not require symmetry *per se* to lay out the atoms and bonds, but rather lays out atoms and bonds that are determined (identified) to be symmetric; when displayed, this constitutes the "visual expression". Using symmetry to layout the atoms/bonds is disclosed in, for example, lines 1-18 of page 9, and line 19, page 9 to line 11, page 10 of the specification. Such an approach is required in order to reposition the atoms/bonds in accordance with the 'stylized' layout, in the sense as argued. Nothing in amended claim 1 requires repositioning to carry out the stylizing. As amended, it is

interpreted that 'stylized representation' is disclosed in the art as the 'displaying' per se teachings.

Claim Rejections - 35 USC § 103

4. The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

> (a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negatived by the manner in which the invention was made.

5. The factual inquiries set forth in *Graham* **v.** *John Deere Co.*, 383 U.S. 1, 148 USPQ 459 (1966), that are applied for establishing a background for determining obviousness under 35 U.S.C. 103(a) are summarized as follows:

1. Determining the scope and contents of the prior art.
2. Ascertaining the differences between the prior art and the claims at issue.
3. Resolving the level of ordinary skill in the pertinent art.
4. Considering objective evidence present in the application indicating obviousness or nonobviousness.

6. Claims 1, 9, 13-35 are rejected under 35 U.S.C. 103(a) as being unpatentable over Helson (The inventor's PhD thesis - of record) in view of Benecke et al. (Applicant's IDS) and the taking of official notice.

7. Helson discloses:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure (pp, 145-149; fig. 4.5; chapter 4; fig. 3.5, pg. 221, fig. 4.9, fig. 5.4);

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds (page 246; fig. 4.5; chapter 4, fig. 4.9, 5.4);

positioning atoms and bonds in the chemical structure diagram pp. 145-149; page 246; fig. 4.5; chapter 3).

Note page 203-211 (redrawing)

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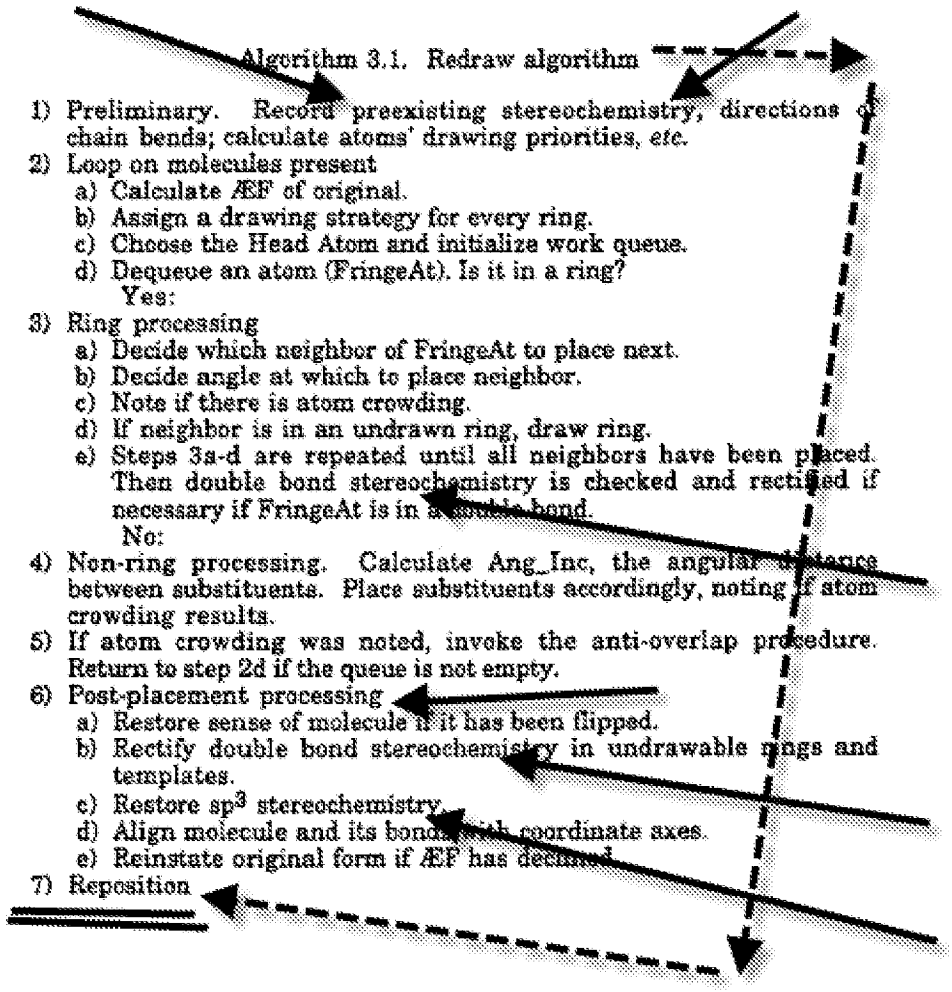
Table 3.1. Criteria for Aef_Redraw

Criterion	Weight*	Description
1	12	Bond overlap
2	3	Bond alignment
3	2	Angle alignment
4	8	Bond distribution
5	4	Alignment and zigzag of chains
6	2	Alignment of ring bonds
7	4	Macroorientation of ring systems
8	6	Symmetry
9	8	Uniform bond length
10	12	Atom crowding

*When a criterion is not applicable to a molecule its weight is set to zero. Similarly, the weights for criteria 5, 6 and 7 are adjusted to reflect the importance of the criterion to the molecule at hand.

And (pg. 149):



Algorithm 3.1. Redraw algorithm

1) Preliminary. Record preexisting stereochemistry, directions of chain bends; calculate atoms' drawing priorities, *etc.*
2) Loop on molecules present
   a) Calculate ÆF of original.
   b) Assign a drawing strategy for every ring.
   c) Choose the Head Atom and initialize work queue.
   d) Dequeue an atom (FringeAt). Is it in a ring?
      Yes:
3) Ring processing
   a) Decide which neighbor of FringeAt to place next.
   b) Decide angle at which to place neighbor.
   c) Note if there is atom crowding.
   d) If neighbor is in an undrawn ring, draw ring.
   e) Steps 3a-d are repeated until all neighbors have been placed. Then double bond stereochemistry is checked and rectified if necessary if FringeAt is in a double bond.
      No:
4) Non-ring processing. Calculate Ang_Inc, the angular difference between substituents. Place substituents accordingly, noting if atom crowding results.
5) If atom crowding was noted, invoke the anti-overlap procedure. Return to step 2d if the queue is not empty.
6) Post-placement processing
   a) Restore sense of molecule if it has been flipped.
   b) Rectify double bond stereochemistry in undrawable rings and templates.
   c) Restore sp^3 stereochemistry.
   d) Align molecule and its bonds with coordinate axes.
   e) Reinstate original form if ÆF has declined.
7) Reposition

8. Note that the redraw algorithm calls the **reposition algorithm**. See page 145-146:

Implementation in CAMEO

In CAMEO, SDG is divided into two independent processes: SDG proper, referred to as "redrawing," and positioning of the resulting molecules, called "repositioning." Both facilities exist as independent packages of routines that may be called to serve different occasions; they are not rigidly tied to any particular phase of the program. In fact, repositioning does not even require perception, although redrawing does. The two executive

routines are REDRAW for SDG proper, and ANA_REPO for positioning. At present REDRAW, which always invokes ANA_REPO at its end, is called from the following places:

Also see the table of contents:

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9. Helson does not appear to disclose

laying out atoms/bonds <u>*to express the identified symmetry*</u> as previously argued by Applicants.

10. Benecke et al. discloses laying out atoms/bonds to express the identified symmetry (pg. 145):

> Each of the structural isomers may exist in several configurations in space. MOLGEN$^+$ is capable of generating all possible configurational isomers, again redundancy free (which, of course, also implies the consideration of symmetries).
>
> The notion stereoisomerism is not uniquely defined in chemistry; it should therefore be stated which kinds of effects are taken into account. Primarily there are: (i) chirality of tetravalent atoms, even in rings and spiranes, and (ii) enantiomerism and diastereomerism of allenes including *cis/trans*-isomerism.

> The construction of the stereoisomers is performed in two steps: First the molecular graph is examined for stereochemical properties and the complete set of configurational isomers is generated without any use of three-dimensional information. This method is based on [6], improved by [9]. Table 2 shows the numbers of stereoisomers corresponding to all structural isomers of a single gross formula.
>
> In the second step spatial realizations of these isomers are calculated by the application of appropriate geometrical transformations to the placement computed above. (The basics of these calculations, which are again discussed in [7], can be found in [8].) In Fig. 2 the four stereoisomers of 1,2,3,4-tetramethylcyclobutane are displayed as an example.

11. It would have been obvious to one of ordinary skill in the art at the time of the invention to so modify Helson in order to generate all configurations to facilitate chemical research.

12. As for dependent claims, Benecke et al. discloses (pg. 45):

> Each of the structural isomers may exist in several configurations in space. MOLGEN$^+$ is capable of generating all possible configurational isomers, again redundancy free (which, of course, also implies the consideration of symmetries).
>
> The notion stereoisomerism is not uniquely defined in chemistry; it should therefore be stated which kinds of effects are taken into account. Primarily there are: (i) chirality of tetravalent atoms, even in rings and spiranes, and (ii) enantiomerism and diastereomerism of allenes including *cis/trans*-isomerism.

Official notice is taken that a skilled artisan would understand that there are a limited group of possible symmetries and would employ them as appropriate. Also, see (Helson) chapter 4 (examples of symmetry).

Allowable Material

13. A novel method appears to be disclosed on lines 2-16, page 11 (force field directed approach). Details of the approach are disclosed on line 17, pg. 11 to line 12, pg. 13. Such an approach is required in order to repositions the atoms/bonds in accordance with the 'stylized' layout, as argued.

Response to Arguments

14. Applicant's arguments, filed 3/2/2010, have been carefully considered and are not persuasive.

15. Applicants appears to argue (remarks and affidavit) unclaimed features. Claim 1, for example, only requires:

> 1. (currently amended) A computer-implemented method for use in deriving a chemical structure diagram, comprising:
>
> identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;
>
> wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;
>
> laying out symmetrically equivalent atoms and bonds in the chemical structure diagram to visually express the identified symmetry in a stylized two-dimensional pictorial representation of the chemical structure; and
>
> outputting [[a]]the pictorial representation of the chemical structure.

The claim does not specify any special meaning to 'stylized'. The claim does not require symmetry *per se* to lay out the atoms and bonds, but rather lays out atoms and bonds that are determined (identified) to be symmetric; when displayed, this constitutes the visual expression. Using symmetry to layout the atoms/bonds is disclosed in, for example, lines 1-18 of page 9, and line 19, page 9 to line 11, page 10 of the specification. A novel method appears to be disclosed on lines 2-16, page 11 (force field directed approach). Details of the approach are disclosed on line 17, pg. 11 to line 12, pg. 13. An approach such as that is required in order to repositions the atoms/bonds in accordance with the 'stylized' layout, as claimed. Nothing in amended claim 1 requires repositioning to carry out the stylizing.

16. *Laying out the symmetrically equivalent atoms and bonds* by itself means that the symmetries are expressed. The claims do not require that the results be aesthetically pleasing.

17. Applicants are thanked for providing the specific reference to the location in the 86 page Helson paper for the teaching regarding 'includes...symmetry as a 'future' advance..".

Conclusion

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Hugh Jones whose telephone number is (571) 272-3781. The examiner can normally be reached on M-Th.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Kamini Shah can be reached on (571) 272-2279. The fax phone number for the organization where this application or proceeding is assigned is 571-273-8300.

Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained

from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see http://pair-direct.uspto.gov. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free). If you would like assistance from a USPTO Customer Service Representative or access to the automated information system, call 800-786-9199 (IN USA OR CANADA) or 571-272-1000.

/Hugh Jones/

Primary Examiner, Art Unit 2128